

Summary of April, 1992 Langley Workshop Recommendations

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(See Table summarizing Spectroscopic Databases starting on page 2)

- Weak lines of the major species (H_2O , CO_2 , O_3 , N_2O , CO , and CH_4) should be better characterized (positions, intensities, assignments, and broadening coefficients). Improved calculations and measurements of broadening coefficients for high-J lines of nonlinear polyatomic molecules such as H_2O , O_3 , and CH_4 are especially needed.
 - Additional investigations of line-mixing are needed for many atmospheric molecules. Theoretical representation of line mixing also needs further work.
 - More pressure-induced line shift measurements are needed for analysis of ground-based atmospheric measurements and for verification of broadening/shift theory.
 - More measurements of line parameters in the far-IR ($\sim 100\text{-}600 \text{ cm}^{-1}$) are needed for many species of interest.
 - Continuum spectra (N_2 , O_2 , H_2O) and non-Lorentzian or non-Voigt line shapes need to be well-characterized, especially for the major gases.
 - The stratospheric aerosol continuum and H_2SO_4 parameters need further study.
 - High-resolution (0.003 to 0.01 cm^{-1}) temperature-dependent cross sections are needed for CFC's and other heavy molecules (e.g., ClONO_2 , N_2O_5 , SF_6) in air at stratospheric to tropospheric pressures.
 - Infrared data for CFC substitutes (present and proposed) and their degradation products is needed at higher resolution than presently available (usually 5-10 cm^{-1}), and at atmospheric pressures and temperatures.
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Summary of Spectroscopic Databases

| Species | Spectral Interval ^a | Intensity Range ^b | Number of Transitions | Quality ^c Database ^d | | | | | Comments ^e |
|------------------|--------------------------------|------------------------------|-----------------------|--|---|----------|---|---|--|
| | | | | v | S | γ | H | J | |
| H ₂ O | 0-500 | -32, -18 | 49,000 | A | B | B | x | x | Better precision needed due to interference with other species; $\square\Delta K\square > 2$ lines need improvement; γ beyond J = 8; SB, <i>n</i> , shifts; line shapes and continua |
| | 500-2200 | | | A | B | B | x | | |
| | 2200-5000 | -27, -19 | | B | B | B | x | | |
| | 5000-23000 | -27, -20 | | B | B | B | x | | |
| CO ₂ | 400-1400 | -27, -19 | 60,000 | A | B | A | x | | More strengths to $\pm 1\%$ needed for p, T retrievals; v, S need improvement for isotopic bands and near-IR bands; SB, <i>n</i> ; line mixing |
| | 1800-2400 | -37, -18 | | A | B | A | x | | |
| | 2400-9700 | -27, -20 | | A | B | A | x | | |
| O ₃ | 0-300 | -26, -21 | 140,000 | A | B | B | x | x | Better precision needed due to interference with other species; Need to add 2.7 μm and 2.5 μm bands, and some isotopic and hot bands; More γ , <i>n</i> , shifts, and SB, especially at high K _a |
| | 300-500 | | | A | B | B | x | | |
| | 500-1200 | -25, -20 | | A | B | B | x | | |
| | 1600-2900 | -26, -21 | | B | B | B | x | | |
| | 2900-3200 | -26, -21 | | B | B | B | x | | |
| N ₂ O | 0-50 | -25, -22 | 16,000 | A | A | A | x | x | γ 's, <i>n</i> 's need verification; SB |
| | 500-1400 | -24, -19 | | A | A | A | x | | |
| | 1600-2900 | -24, -19 | | A | A | A | x | | |
| | 2900-5000 | -24, -19 | | B | B | A | x | | |
| CO | 0-150 | -24, -21 | 3,600 | A | A | A | x | x | Parameters in 150-200 cm^{-1} region should be added; SB, <i>n</i> |
| | 1900-6400 | -24, -19 | | A | A | B | x | | |

Summary of Spectroscopic Databases (Cont'd)

| Species | Spectral Interval ^a | Intensity Range ^b | Number of Transitions | Quality ^c Database ^d | | | | | Comments ^e |
|---------------------------------------|--------------------------------|------------------------------|-----------------------|--|---|----------|---|---|---|
| | | | | v | S | γ | H | J | |
| CH ₄ and CH ₃ D | 0-100 | -29, -27 | 47,000 | A | A | A | x | x | Some hot bands missing; More measured γ 's, n's, shifts needed; 5000-5500 cm ⁻¹ , 7100-7800 cm ⁻¹ regions missing; add at least an average shift coefficient for each region |
| | 900-2000 | -29, -19 | | A | A | B | x | | |
| | 2200-3200 | -40, -19 | | A | B | B | x | | |
| | 4100-7800 | -23, -20 | | C | C | B | x | | |
| O ₂ | 0-300 | -35, -25 | 2,200 | A | A | C | x | x | S for rotational lines should be checked and revisions made; Add pressure-induced bands |
| | 1400-16000 | -30, -23 | | A | B | B | x | | |
| N ₂ | 2000-2600 | -34, -28 | 100 | A | A | B | x | | Add pressure-induced bands |
| O | 68-158 | -22, -21 | 2 | A | A | | | x | |
| NO | 0-130 | -35, -22 | 7,400 | A | A | B | x | x | Need cross-ladder rotational transitions; Include IR hyperfine structure; Need measured γ 's by air; SB |
| | 1500-4000 | -44, -19 | | A | B | B | x | | |
| NO ₂ | 0-330 | -25, -20 | 55,000 | A | A | | | x | Add JPL catalogue data to HITRAN; Incorporate recent IR v, S results from R.Toth and A. Perrin; SB |
| | 600-3000 | -24, -19 | | A | B | B | x | | |
| NH ₃ | 0-400 | -29, -21 | 7,000 | A | A | B | x | x | 6 μ m region needs revision; 3 μ m region needed |
| | 400-2200 | -28, -29 | | B | B | B | x | | |

Summary of Spectroscopic Databases (Cont'd)

| Species | Spectral Interval ^a | Intensity Range ^b | Number of Transitions | Quality ^c Database ^d | | | | | Comments ^e |
|------------------------|---|------------------------------|-----------------------|--|---|----------|---|---|---|
| | | | | v | S | γ | H | J | |
| HNO_3 | 0-100 | -26, -21 | 143,000 | A | A | C | x | x | Microwave γ 's from DeLucia should be added; Bands at 3550 cm^{-1} needed; nearly all hot bands needed |
| | 390-?(v ₉) | -23, -17 | | A | B | C | x | | |
| | (v ₆) | -23, -18 | | A | B | C | x | | |
| | (v ₇) | -23, -19 | | A | B | C | x | | |
| | (v ₈) | -23, -18 | | A | B | C | x | | |
| | (v ₅ , 2v ₉ , h.b.) | -23, -17 | | B | B | C | x | | |
| | (v ₈ +v ₉) | -23, -18 | | A | B | C | x | | |
| | (v ₃ , v ₄) | -23, -17 | | B | C | C | x | | |
| | ?-1750(v ₂) | -23, -17 | | A | B | C | x | | |
| HCN | 0-150 | -24, -18 | 800 | A | A | B | x | x | SB; <i>n</i> |
| | 550-3450 | -25, -19 | | A | A | B | x | | |
| N_2O_5 | 555-1765 | CS | | B | B | C | x | | Need measurements at T < 230K, if possible Add new Giessen data for $350-650 \text{ cm}^{-1}$ region |
| HNO_4 | 0-? | | ? | - | - | | - | - | Incomplete data; need more pressures and temperatures |
| | 770-830 | CS | | C | C | C | x | | |
| OH | 0-200 | -31, -18 | 8,500 | A | A | B | x | x | Excited-state rotational lines needed; New extended vibration-rotation prediction forthcoming |
| | 1250-10000 | -81, -19 | | A | B | C | x | | |
| HO_2 | 0-100 | -25, -20 | 6,200 | A | A | | x | | Add JPL catalogue parameters to HITRAN; Add IR fundamental parameters from Zahniser |

Summary of Spectroscopic Databases (Cont'd)

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|------------------------|--------------------------------|------------------------------|-----------------------|--|---|----------|---|---|---|
| | | | | v | S | γ | H | J | |
| H_2O_2 | 0-300 | -26, -20 | 5,400 | A | A | A | x | x | Rotational bands need update on HITRAN; Only one IR band at present; 3 μm region needed |
| | 1150-1350 | -23, -20 | | A | B | B | x | | |
| HCl | 0-400 | -24, -18 | 400 | A | A | B | x | x | Quadrupole rotational lines needed on HITRAN |
| | 2400-8500 | -24, -19 | | A | A | A | x | | |
| HF | 0-250 | -24, -17 | 110 | A | A | B | x | x | SB T-dependence |
| | 250-8000 | -24, -17 | | A | A | A | x | | |
| HBr | 0-350 | -24, -18 | 400 | A | A | A | x | x | Quadrupole rotational lines needed on HITRAN |
| | 2200-9800 | -24, -19 | | A | A | B | x | | |
| HI | 0-8500 | -24, -18 | 400 | A | A | A | x | | |
| ClO | 0-100 | -29, -21 | 6,000 | A | A | B | x | x | Need cross-ladder rotational transitions 300-335 cm^{-1} and spin-orbit transitions near 318 cm^{-1} ; 1-0 intensities need to be updated |
| | 300-350 | ?, ? | | - | - | - | | | |
| | 760-900 | -24, -20 | | A | C | B | x | | |
| OCIO | 0-100 | ?, ? | ? | - | - | - | | x | Add IR transitions |
| ClOOCl | 0-30 | ?, ? | ? | - | - | - | | x | Add IR transitions |
| HOCl | 0-300 | -26, -19 | 15,600 | A | A | A | | x | Missing fundamental should be added; ν_1 to be revised |
| | 1150-3800 | -23, -20 | | A | B | C | x | | |
| BrO | 0-100 | ?, ? | ? | A | A | B | | x | |

Summary of Spectroscopic Databases (Cont'd)

| Species | Spectral Interval ^a | Intensity Range ^b | Number of Transitions | Quality ^c | | | | | Comments ^e |
|--------------------------------|--------------------------------|------------------------------|-----------------------|----------------------|--------|----------|--------|---|---|
| | | | | v | S | γ | H | J | |
| CF ₂ O | 700-2000 | CS | | A | B | B | x | | Some revisions needed |
| SF ₆ | 948-953 | CS | | A | B | B | x | | More bands needed, including hot bands |
| OCS | 0-40 800-2100 | -28, -21 -23, -18 | 700 | A B | A B | B | x x | x | 100-300 cm ⁻¹ region needed; 3.4 μ m and 2.4 μ m bands on GEISA should be evaluated for addition to HITRAN |
| SO ₂ | 0-200 400-2550 | -24, -20 -23, -19 | 26,000 | A A | A B | C | x x | x | More γ 's needed; SB (large); Region > 5000 cm ⁻¹ of planetary interest |
| H ₂ S | 0-600 900-1600 | -27, -19 -23, -21 | 600 | A A | A A | C | x x | x | Missing some fundamentals; incorporate available data from GEISA |
| H ₂ SO ₄ | 0-10 | - | - | A | B | | | x | More measurements at higher frequencies needed |
| C ₂ H ₂ | 600-3400 | -25, -18 | 1,300 | A | A | B | x | | NIST 3 μ m parameters should be added; 720 cm ⁻¹ region needed from GEISA |
| C ₂ H ₄ | - | - | - | - | - | - | - | - | Consider adding 900-1100 cm ⁻¹ GEISA data to HITRAN |
| C ₂ H ₆ | 700-3000 | -25, -21 | 4,700 | C | C | C | x | | Improvements required in 3 μ m region |
| C ₃ H ₈ | - | - | - | - | - | - | - | - | Consider adding to HITRAN |

Summary of Spectroscopic Databases (Cont'd)

| Species | Spectral Interval ^a | Intensity Range ^b | Number of Transitions | Quality ^c Database ^d | | | | | Comments ^e |
|---|--------------------------------|------------------------------|-----------------------|--|---|----------|---|---|--|
| | | | | v | S | γ | H | J | |
| H ₂ CO | 0-100 | -38, -19 | 2,700 | A | A | C | x | x | Add GEISA data 1060-1160 cm ⁻¹ to HITRAN |
| | 2700-3000 | -20, -19 | | A | A | C | x | | |
| HCOOH | 0-100 | -28, -21 | 1888 | B | A | C | | x | Add GEISA data 1060-1160 cm ⁻¹ to HITRAN |
| CH ₃ Cl | 2900-3200 | -25, -21 | 6,700 | B | B | C | x | | Need v ₁ Q ₇ and Q ₈ , and v ₃ |
| CCl ₄ | | CS | | | | | x | | |
| CFCl ₃ (CFC-11) | | CS | | | | | x | | |
| CF ₂ Cl ₂ (CFC-12) | | CS | | | | | x | | |
| CF ₃ Cl (CFC-13) | | CS | | | | | x | | |
| CF ₄ (CFC-14) | | CS | | | | | x | | |
| CHCl ₂ F (HCFC-21) | | CS | | | | | x | | |
| CHClF ₂ (HCFC-22) | | CS | | | | | x | | New NIST low-T data to be considered |

Summary of Spectroscopic Databases (Cont'd)

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|--|--------------------------------|------------------------------|-----------------------|----------------------|---|----------|-----------------------|---|--------------------------------------|
| | | | | v | S | γ | H | J | |
| CHF ₃ (HCFC-23) | | | | | | - | | | Add rotational and IR data available |
| C ₂ Cl ₃ F ₃ (CFC-113) | | CS | | | | x | | | |
| C ₂ Cl ₂ F ₄ (CFC-114) | | CS | | | | x | | | |
| C ₂ ClF ₅ (CFC-115) | | CS | | | | x | | | |
| CH ₃ CF ₃ (HCFC-143a) | | | | | | - | | | Add rotational and IR data available |
| CH ₃ CCl ₃ (methyl chloroform) | | | | | | - | | | Add rotational and IR data available |

^aSpectral intervals are given in units of cm⁻¹ (100 μ m wavelength \square 100 cm⁻¹ wavenumber \square 3 THz frequency).

^bIntensity range is given as the log of the minimum and maximum line intensities in units of cm⁻¹/(molecule cm⁻²). The abbreviation "CS" indicates that only absorption cross-sections are available in the databases.

^cThe quality codes indicate: A, good for most applications; B, good for some applications but needs some improvements; C, needs major improvements. The three columns refer to line position (v), line intensity (S), and air-broadening coefficient (γ).

^dDatabase codes are: H, HITRAN (1992); J, JPL (1991) catalog.

^eThe need for self-broadening coefficients is abbreviated as "SB", and the need for measurements of the temperature dependence of air-broadening coefficients is indicated by "n".

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